


## Message

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**Subject:** RE: PFAS chemicals retrieved from various data systems

Colleagues,

Looking through the spreadsheet I think one of the most important questions for this group is the distinction between the salt forms and the acid forms. People are using PFOS to refer to BOTH perfluorooctanesulfonate and perfluorooctanesulfonic acid and we deal with this for synonym lookup as shown below.

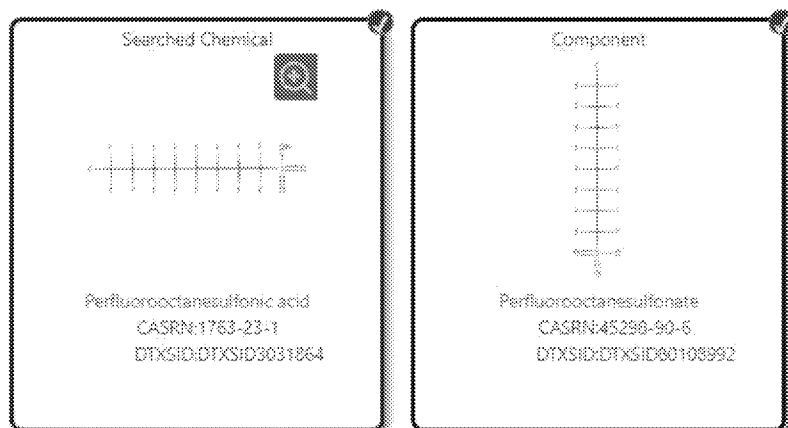


**Chemicals**   Product/Use Categories   Assay/Gene

Q PFOS

- PFOS ion(-1)  
DTXSID00108992
- PFOS-K  
DTXSID0017706
- PFOS-Li  
DTXSID0032421
- PFOSA  
DTXSID0032939
- PFOSaAm  
DTXSID0065443
- PFOSaAmA  
DTXSID0082552
- PFOSNO  
DTXSID00700460
- PFOS  
DTXSID0031864
- PFOS-Na  
DTXSID00635462

But if you SEARCH PFOS we provide the acid: Ex. 6 Personal Privacy (PP)  
 CHEMISTS would think of the ..sulfonate as the CHARGED anion, not the acid, as we do below.



They have distinct CASRNs. The same issue is for all of the “salts” and “acids” below. There are distinct CASRNs for the anions, the individual salt forms (K<sup>+</sup>, Na<sup>+</sup>, NH<sub>4</sub><sup>+</sup> etc and the acid.

5	Perfluorooctanoic Acid
5	Perfluorobutane Sulfonate
7	Perfluorohexanoic acid
3	Perfluorohexane Sulfonate
3	Perfluoroheptanoic acid
0	Perfluorononanoic acid
1	Perfluorodecanoic acid

For the list above I suggest homogenizing to ALL acids. If you want to include all anionic forms of these acids that can be done also but they should be separate. I believe that consistency across the various lists would be of value so that collisions between PFOS and PFOA, for example are resolved. Look at UCMR3

UCMR 3 - Contaminant	
	perfluorooctanesulfonic acid (PFOS)
	perfluorooctanoic acid (PFOA)
	perfluorononanoic acid (PFNA)
	perfluorohexanesulfonic acid (PFHxS)
	perfluoroheptanoic acid (PFHpA)
	perfluorobutanesulfonic acid (PFBS)

Versus POI

6	Perfluorooctanoic Acid (PFOA)
7	Perfluorononanoic Acid (PFNA)
8	Perfluorooctane Sulfonate (PFOS)

If I can get basic agreement on this the lists can be mapped together for consistency and handed back. Thanks

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Try out the [CompTox Chemicals Dashboard](#) and access data for almost 875,000 chemical substances

**HOT OFF THE PRESS** ["Open-source QSAR models for pKa prediction using multiple machine learning approaches"](#)

**From:** Andrew Stoeckle <Andrew.Stoeckle@erg.com>

**Sent:** Monday, January 20, 2020 5:35 PM

**To:** Buckley, Timothy <Buckley.Timothy@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; Pilant, Drew <Pilant.Drew@epa.gov>; Scheitlin, Tom <Scheitlin.Tom@epa.gov>; Neale, Anne <Neale.Anne@epa.gov>; Giri, Chandra <Giri.Chandra@epa.gov>; Hubal, Elaine <Hubal.Elaine@epa.gov>; Linkins, Samantha <Linkins.Samantha@epa.gov>; Tadesse, Haile <tadesse.haile@epa.gov>; Yourish, Jesse <yourish.jesse@epa.gov>; Burden, David <Burden.David@epa.gov>; DeLuca, Nicole <DeLuca.Nicole@epa.gov>; Hanselman, Erik <Hanselman.Erik@epa.gov>; Baxter, Lisa <Baxter.Lisa@epa.gov>; Gillespie, Andrew <Gillespie.Andrew@epa.gov>; Matthew Heyward

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**Subject:** PFAS chemicals retrieved from various data systems

Last week, Antony Williams (NCCT) requested the list of PFAS chemicals that have been retrieved for presentation in the National PFAS Data Explorer.

The most current list for each data system is attached (Thanks Emma). It should be noted, that each data system involves a different method of retrieval and future retrievals may change these lists as:

- the authoritative lists of defined structures and undefined structures may be updated by NCCT,
- records may be added to certain data systems (e.g., Water Quality Portal, DMR Loadings Tool), and
- PFAS flags within data systems may be updated (e.g., DMR Loadings Tool).

Additionally, flow diagrams describing the as-is state and potential future state of PFAS record retrieval for the Water Quality Portal are included in the ppt file.

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